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Employment

2022–…	**Assistant Professor** (Computer Science) University of Antwerp, Antwerp, Belgium
2019–22	**Postdoctoral Researcher** (Pharmacy and Pharmaceutical Sciences) University of California San Diego, La Jolla, CA, USA Advisor: Pieter C. Dorrestein, PhD
2017–19	**Postdoctoral Researcher** (Genome Sciences) University of Washington, Seattle, WA, USA Advisor: William Stafford Noble, PhD

Education

2013–17	**PhD in Computer Science** University of Antwerp, Antwerp, Belgium Thesis: *Computational Solutions for Quality Control of Mass Spectrometry-based Proteomics* Advisors: Kris Laukens, PhD and Bart Goethals, PhD
2016	**Visiting Researcher** Stellenbosch University, Cape Town, South Africa
2010–12	**MSc in Computer Science** Hasselt University, Diepenbeek, Belgium Thesis: *Time Series Similarity Search* Advisors: Marc Gyssens, PhD
2007–10	**BSc in Computer Science** Hasselt University, Diepenbeek, Belgium Thesis: *Extending a Web Browser With Additional Navigation Options* Advisors: Jan Van den Bussche, PhD

Awards and Honors

2023	**Young Investigator Award**, *Metabolites*
2023	**Bioinformatics for Mass Spectrometry Award**, European Proteomics Association
2022	**Early Career Researcher Manuscript Competition Award** Human Proteome Organization
2021	**Rising Stars in Proteomics and Metabolomics: 40 Under 40** *Journal of Proteome Research*
2020	**Postdoctoral Career Development Award**, American Society for Mass Spectrometry
2015	**Best Oral Presentation Award**, Benelux Bioinformatics Conference

Peer-Reviewed Publications

[66] Melih Yilmaz, William E. Fondrie, **Wout Bittremieux**, Carlo F. Melendez, Rowan Nelson, Varun Ananth, Sewoong Oh, and William Stafford Noble. "Sequence-to-Sequence Translation From Mass Spectra to Peptides With a Transformer Model." In: *Nature Communications* (2024), In Press.

[65] Chris Bielow, Nils Hoffmann, David Jimenez-Morales, Tim Van Den Bossche, Juan Antonio Vizcaíno, David L. Tabb, **Wout Bittremieux**, and Mathias Walzer. "Communicating Mass Spectrometry Quality Information in mzQC With Python, R, and Java." In: *Journal of The American Society for Mass Spectrometry* (2024), In Press. DOI: `10.1101/2024.05.06.592686`.

[64] Charlotte Adams, Wassim Gabriel, Kris Laukens, Mario Picciani, Mathias Wilhelm, **Wout Bittremieux**, and Kurt Boonen. "Fragment Ion Intensity Prediction Improves the Identification Rate of Non-Tryptic Peptides in TimsTOF." In: *Nature Communications* 15.1 (May 10, 2024), p. 3956. DOI: `10.1038/s41467-024-48322-0`.

[63] Issar Arab, Kristof Egghe, Kris Laukens, Ke Chen, Khaled Barakat, and **Wout Bittremieux**. "Benchmarking of Small Molecule Feature Representations for hERG, Nav1.5, and Cav1.2 Cardiotoxicity Prediction." In: *Journal of Chemical Information and Modeling* 64.7 (Apr. 8, 2024), pp. 2515–2527. DOI: `10.1021/acs.jcim.3c01301`.

[62] Charlotte Adams, Kris Laukens, **Wout Bittremieux**, and Kurt Boonen. "Machine Learning-Based Peptide-Spectrum Match Rescoring Opens Up the Immunopeptidome." In: *PROTEOMICS* 24.8 (Apr. 2024), p. 2300336. DOI: `10.1002/pmic.202300336`.

[61] Ipsita Mohanty, Helena Mannochio-Russo, Joshua V. Schweer, Yasin El Abiead, **Wout Bittremieux**, Shipei Xing, Robin Schmid, Simone Zuffa, Felipe Vasquez, Valentina B. Muti, Jasmine Zemlin, Omar E. Tovar-Herrera, Sarah Moraïs, Dhimant Desai, Shantu Amin, Imhoi Koo, Christoph W. Turck, Itzhak Mizrahi, Penny M. Kris-Etherton, Kristina S. Petersen, Jennifer A. Fleming, Tao Huan, Andrew D. Patterson, Dionicio Siegel, Lee R. Hagey, Mingxun Wang, Allegra T. Aron, and Pieter C. Dorrestein. "The Underappreciated Diversity of Bile Acid Modifications." In: *Cell* 187.7 (Mar. 28, 2024), 1801–1818.e20. DOI: `10.1016/j.cell.2024.02.019`.

[60] Jaeyoung Kang, Weihong Xu, **Wout Bittremieux**, Niema Moshiri, and Tajana Rosing. "DRAM-Based Acceleration of Open Modification Search in Hyperdimensional Space." In: *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems* (Mar. 28, 2024), Early Access. DOI: `10.1109/TCAD.2024.3382842`.

[59] Sumukh Pinge, Weihong Xu, Jaeyoung Kang, Tianqi Zhang, Neima Moshiri, **Wout Bittremieux**, and Tajana Rosing. "SpecHD: Hyperdimensional Computing Framework for FPGA-based Mass Spectrometry Clustering." In: *Proceedings of the 2024 Design, Automation & Test in Europe Conference - DATE 2024*. Valencia, Spain, Mar. 25, 2024. DOI: `10.48550/arXiv.2311.12874`.

[58] **Wout Bittremieux**, Nicole E. Avalon, Sydney P. Thomas, Sarvar A. Kakhkhorov, Alexander A. Aksenov, Paulo Wender P. Gomes, Christine M. Aceves, Andrés Mauricio Caraballo-Rodríguez, Julia M. Gauglitz, William H. Gerwick, Tao Huan, Alan K. Jarmusch, Rima F. Kaddurah-Daouk, Kyo Bin Kang, Hyun Woo Kim, Todor Kondić, Helena Mannochio-Russo, Michael J. Meehan, Alexey V. Melnik, Louis-Felix Nothias, Claire O'Donovan, Morgan Panitchpakdi, Daniel Petras, Robin Schmid, Emma L. Schymanski, Justin J. J. Van Der Hooft, Kelly C. Weldon, Heejung Yang, Shipei Xing, Jasmine Zemlin, Mingxun Wang, and Pieter C. Dorrestein. "Open Access Repository-Scale Propagated Nearest Neighbor Suspect Spectral Library For Untargeted Metabolomics." In: *Nature Communications* 14.1 (Dec. 20, 2023), p. 8488. DOI: `10.1038/s41467-023-44035-y`.

[57] Ceder Dens, Kris Laukens, **Wout Bittremieux**, and Pieter Meysman. "The Pitfalls of Negative Data Bias For the T-cell Epitope Specificity Challenge." In: *Nature Machine Intelligence* 5 (Oct. 2023), pp. 1060–1062. DOI: `10.1038/s42256-023-00727-0`.

[56] Ceder Dens, **Wout Bittremieux**, Fabio Affaticati, Kris Laukens, and Pieter Meysman. "Interpretable Deep Learning to Uncover the Molecular Binding Patterns Determining TCR–Epitope Interaction Predictions." In: *ImmunoInformatics* 11 (Sept. 2023), p. 100027. DOI: `10.1016/j.immuno.2023.100027`.

[55] Jaeyoung Kang, Weihong Xu, **Wout Bittremieux**, Niema Moshiri, and Tajana Rosing. "Accelerating Open Modification Spectral Library Searching on Tensor Core in High-Dimensional Space." In: *Bioinformatics* 39.7 (June 27, 2023). Ed. by Janet Kelso, btad404. DOI: `10.1093/bioinformatics/btad404`.

[54] Weihong Xu, Jaeyoung Kang, **Wout Bittremieux**, Niema Moshiri, and Tajana Rosing. "HyperSpec: Ultrafast Mass Spectra Clustering in Hyperdimensional Space." In: *Journal of Proteome Research* (May 11, 2023). DOI: 10.1021/acs.jproteome.2c00612.

[53] **Wout Bittremieux**, Lev Levitsky, Matteo Pilz, Timo Sachsenberg, Florian Huber, Mingxun Wang, and Pieter C. Dorrestein. "Unified and Standardized Mass Spectrometry Data Processing in Python Using spectrum_utils." In: *Journal of Proteome Research* 22.2 (Feb. 3, 2023), pp. 625–631. DOI: 10.1021/acs.jproteome.2c00632.

[52] Issar Arab, William E. Fondrie, Kris Laukens, and **Wout Bittremieux**. "Semisupervised Machine Learning for Sensitive Open Modification Spectral Library Searching." In: *Journal of Proteome Research* 22.2 (Feb. 3, 2023), pp. 585–593. DOI: 10.1021/acs.jproteome.2c00616.

[51] Eric W. Deutsch, Juan Antonio Vizcaíno, Andrew R. Jones, Pierre-Alain Binz, Henry Lam, Joshua Klein, **Wout Bittremieux**, Yasset Perez-Riverol, David L. Tabb, Mathias Walzer, Sylvie Ricard-Blum, Henning Hermjakob, Steffen Neumann, Tytus D. Mak, Shin Kawano, Luis Mendoza, Tim Van Den Bossche, Ralf Gabriels, Nuno Bandeira, Jeremy Carver, Benjamin Pullman, Zhi Sun, Nils Hoffmann, Jim Shofstahl, Yunping Zhu, Luana Licata, Federica Quaglia, Silvio C. E. Tosatto, and Sandra E. Orchard. "Proteomics Standards Initiative at Twenty Years: Current Activities and Future Work." In: *Journal of Proteome Research* 22.2 (Feb. 3, 2023), pp. 287–301. DOI: 10.1021/acs.jproteome.2c00637.

[50] Julia M. Gauglitz, Kiana A. West, **Wout Bittremieux**, Candace L. Williams, Kelly C. Weldon, Morgan Panitchpakdi, Francesca Di Ottavio, Christine M. Aceves, Elizabeth Brown, Nicole C. Sikora, Alan K. Jarmusch, Cameron Martino, Anupriya Tripathi, Michael J. Meehan, Kathleen Dorrestein, Justin P. Shaffer, Roxana Coras, Fernando Vargas, Lindsay DeRight Goldasich, Tara Schwartz, MacKenzie Bryant, Gregory Humphrey, Abigail J. Johnson, Katharina Spengler, Pedro Belda-Ferre, Edgar Diaz, Daniel McDonald, Qiyun Zhu, Emmanuel O. Elijah, Mingxun Wang, Clarisse Marotz, Kate E. Sprecher, Daniela Vargas-Robles, Dana Withrow, Gail Ackermann, Lourdes Herrera, Barry J. Bradford, Lucas Maciel Mauriz Marques, Juliano Geraldo Amaral, Rodrigo Moreira Silva, Flavio Protasio Veras, Thiago Mattar Cunha, Rene Donizeti Ribeiro Oliveira, Paulo Louzada-Junior, Robert H. Mills, Paulina K. Piotrowski, Stephanie L. Servetas, Sandra M. Da Silva, Christina M. Jones, Nancy J. Lin, Katrice A. Lippa, Scott A. Jackson, Rima Kaddurah Daouk, Douglas Galasko, Parambir S. Dulai, Tatyana I. Kalashnikova, Curt Wittenberg, Robert Terkeltaub, Megan M. Doty, Jae H. Kim, Kyung E. Rhee, Julia Beauchamp-Walters, Kenneth P. Wright, Maria Gloria Dominguez-Bello, Mark Manary, Michelli F. Oliveira, Brigid S. Boland, Norberto Peporine Lopes, Monica Guma, Austin D. Swafford, Rachel J. Dutton, Rob Knight, and Pieter C. Dorrestein. "Enhancing Untargeted Metabolomics Using Metadata-Based Source Annotation." In: *Nature Biotechnology* 40 (Dec. 2022), pp. 1774–1779. DOI: 10.1038/s41587-022-01368-1.

[49] Justin P. Shaffer, Louis-Félix Nothias, Luke R. Thompson, Jon G. Sanders, Rodolfo A. Salido, Sneha P. Couvillion, Asker D. Brejnrod, Franck Lejzerowicz, Niina Haiminen, Shi Huang, Holly L. Lutz, Qiyun Zhu, Cameron Martino, James T. Morton, Smruthi Karthikeyan, Mélissa Nothias-Esposito, Kai Dührkop, Sebastian Böcker, Hyun Woo Kim, Alexander A. Aksenov, **Wout Bittremieux**, Jeremiah J. Minich, Clarisse Marotz, MacKenzie M. Bryant, Karenina Sanders, Tara Schwartz, Greg Humphrey, Yoshiki Vásquez-Baeza, Anupriya Tripathi, Laxmi Parida, Anna Paola Carrieri, Kristen L. Beck, Promi Das, Antonio González, Daniel McDonald, Joshua Ladau, Søren M. Karst, Mads Albertsen, Gail Ackermann, Jeff DeReus, Torsten Thomas, Daniel Petras, Ashley Shade, James Stegen, Se Jin Song, Thomas O. Metz, Austin D. Swafford, Pieter C. Dorrestein, Janet K. Jansson, Jack A. Gilbert, Rob Knight, the Earth Microbiome Project 500 (EMP500) Consortium, Lars T. Angenant, Alison M. Berry, Leonora S. Bittleston, Jennifer L. Bowen, Max Chavarría, Don A. Cowan, Dan Distel, Peter R. Girguis, Jaime Huerta-Cepas, Paul R. Jensen, Lingjing Jiang, Gary M. King, Anton Lavrinienko, Aurora MacRae-Crerar, Thulani P. Makhalanyane, Tapio Mappes, Ezequiel M. Marzinelli, Gregory Mayer, Katherine D. McMahon, Jessica L. Metcalf, Sou Miyake, Timothy A. Mousseau, Catalina Murillo-Cruz, David Myrold, Brian Palenik, Adrián A. Pinto-Tomás, Dorota L. Porazinska, Jean-Baptiste Ramond, Forest Rowher, Taniya RoyChowdhury, Stuart A. Sandin, Steven K. Schmidt, Henning Seedorf, Ashley Shade, J. Reuben Shipway, Jennifer E. Smith, James Stegen, Frank J. Stewart, Karen Tait, Torsten Thomas, Yael Tucker, Jana M. U'Ren, Phillip C. Watts, Nicole S. Webster, Jesse R. Zaneveld, and Shan Zhang. "Standardized Multi-Omics of Earth's Microbiomes Reveals Microbial and Metabolite Diversity." In: *Nature Microbiology* 7.12 (Nov. 28, 2022), pp. 2128–2150. DOI: 10.1038/s41564-022-01266-x.

[48] **Wout Bittremieux**, Mingxun Wang, and Pieter C. Dorrestein. "The Critical Role That Spectral Libraries Play in Capturing the Metabolomics Community Knowledge." In: *Metabolomics* 18.94 (Nov. 19, 2022). DOI: `10.1007/s11306-022-01947-y`.

[47] Charlotte Adams, Kurt Boonen, Kris Laukens, and **Wout Bittremieux**. "Open Modification Searching of SARS-CoV-2–Human Protein Interaction Data Reveals Novel Viral Modification Sites." In: *Molecular & Cellular Proteomics* 21.12 (Oct. 2022), p. 100425. DOI: `10.1016/j.mcpro.2022.100425`.

[46] Bart Cuypers, Pieter Meysman, Ionas Erb, **Wout Bittremieux**, Dirk Valkenborg, Geert Baggerman, Inge Mertens, Shyam Sundar, Basudha Khanal, Cedric Notredame, Jean-Claude Dujardin, Malgorzata A. Domagalska, and Kris Laukens. "Four Layer Multi-Omics Reveals Molecular Responses to Aneuploidy in Leishmania." In: *PLOS Pathogens* 18.9 (Sept. 23, 2022), e1010848. DOI: `10.1371/journal.ppat.1010848`.

[45] **Wout Bittremieux**, Robin Schmid, Florian Huber, Justin J.J. van der Hooft, Mingxun Wang, and Pieter C. Dorrestein. "Comparison of Cosine, Modified Cosine, and Neutral Loss Based Spectrum Alignment For Discovery of Structurally Related Molecules." In: *Journal of The American Society for Mass Spectrometry* 33.9 (Sept. 7, 2022), pp. 1733–1744. DOI: `10.1021/jasms.2c00153`.

[44] Raphael Reher, Allegra T. Aron, Pavla Fajtová, Paolo Stincone, Berenike Wagner, Alicia I. Pérez-Lorente, Chenxi Liu, Ido Y. Ben Shalom, **Wout Bittremieux**, Mingxun Wang, Kyowon Jeong, Marie L. Matos-Hernandez, Kelsey L. Alexander, Eduardo J. Caro-Diaz, C. Benjamin Naman, J. H. William Scanlan, Phil M. M. Hochban, Wibke E. Diederich, Carlos Molina-Santiago, Diego Romero, Khaled A. Selim, Peter Sass, Heike Brötz-Oesterhelt, Chambers C. Hughes, Pieter C. Dorrestein, Anthony J. O'Donoghue, William H. Gerwick, and Daniel Petras. "Native Metabolomics Identifies the Rivulariapeptolide Family of Protease Inhibitors." In: *Nature Communications* 13.1 (Aug. 8, 2022), p. 4619. DOI: `10.1038/s41467-022-32016-6`.

[43] Melih Yilmaz, William E. Fondrie, **Wout Bittremieux**, Sewoong Oh, and William Stafford Noble. "*De Novo* Mass Spectrometry Peptide Sequencing with a Transformer Model." In: *Proceedings of the 39th International Conference on Machine Learning - ICML '22*. Vol. 162. Proceedings of Machine Learning Research. Baltimore, MD, USA: PMLR, July 17, 2022, pp. 25514–25522.

[42] **Wout Bittremieux** and William Stafford Noble. "A Neural Network for Large-Scale Clustering of Peptide Mass Spectra." In: *Nature Methods* 19 (June 2022), pp. 658–659. DOI: `10.1038/s41592-022-01497-0`.

[41] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding For Efficient Joint Analysis of Millions of Mass Spectra." In: *Nature Methods* 19 (June 2022), pp. 675–678. DOI: `10.1038/s41592-022-01496-1`.

[40] Xiyang Luo, **Wout Bittremieux**, Johannes Griss, Eric W. Deutsch, Timo Sachsenberg, Lev I. Levitsky, Mark V. Ivanov, Julia A. Bubis, Ralf Gabriels, Henry Webel, Aniel Sanchez, Mingze Bai, Lukas Käll, and Yasset Perez-Riverol. "A Comprehensive Evaluation of Consensus Spectrum Generation Methods in Proteomics." In: *Journal of Proteome Research* 21.6 (June 3, 2022), pp. 1566–1574. DOI: `10.1021/acs.jproteome.2c00069`.

[39] Richard D. LeDuc, Eric W. Deutsch, Pierre-Alain Binz, Ryan T. Fellers, Anthony J. Cesnik, Joshua A. Klein, Tim Van Den Bossche, Ralf Gabriels, Arshika Yalavarthi, Yasset Perez-Riverol, Jeremy Carver, **Wout Bittremieux**, Shin Kawano, Benjamin Pullman, Nuno Bandeira, Neil L. Kelleher, Paul M. Thomas, and Juan Antonio Vizcaíno. "Proteomics Standards Initiative's ProForma 2.0: Unifying the Encoding of Proteoforms and Peptidoforms." In: *Journal of Proteome Research* 21.4 (Apr. 1, 2022), pp. 1189–1195. DOI: `10.1021/acs.jproteome.1c00771`.

[38] **Wout Bittremieux**, Rohit S Advani, Alan K Jarmusch, Shaden Aguirre, Aileen Lu, Pieter C Dorrestein, and Shirley M Tsunoda. "Physicochemical Properties Determining Drug Detection in Skin." In: *Clinical and Translational Science* 15.3 (Mar. 2022), pp. 761–770. DOI: `10.1111/cts.13198`.

[37] William E Fondrie, **Wout Bittremieux**, and William Stafford Noble. "ppx: Programmatic Access to Proteomics Data Repositories." In: *Journal of Proteome Research* 20.9 (Sept. 3, 2021), pp. 4621–4624. DOI: `10.1021/acs.jproteome.1c00454`.

[36] Eric W Deutsch, Yasset Perez-Riverol, Jeremy Carver, Shin Kawano, Luis Mendoza, Tim Van Den Bossche, Ralf Gabriels, Pierre-Alain Binz, Benjamin Pullman, Zhi Sun, Jim Shofstahl, **Wout Bittremieux**, Tytus Mak, Joshua Klein, Yunping Zhu, Henry Lam, Juan Antonio Vizcaino, and Nuno Bandeira. "Universal Spectrum Identifier For Mass Spectra." In: *Nature Methods* 18 (July 2021), pp. 768–770. DOI: `10.1038/s41592-021-01184-6`.

[35] **Wout Bittremieux**, Kris Laukens, William Stafford Noble, and Pieter C Dorrestein. "Large-Scale Tandem Mass Spectrum Clustering Using Fast Nearest Neighbor Searching." In: *Rapid Communications in Mass Spectrometry* (June 25, 2021), e9153. DOI: 10.1002/rcm.9153.

[34] Youzhong Liu, Thomas De Vijlder, **Wout Bittremieux**, Kris Laukens, and Wouter Heyndrickx. "Current and Future Deep Learning Algorithms for MS/MS-based Small Molecule Structure Elucidation." In: *Rapid Communications in Mass Spectrometry* (May 6, 2021), e9120. DOI: 10.1002/rcm.9120.

[33] **Wout Bittremieux**, David Bouyssié, Viktoria Dorfer, Marie Locard-Paulet, Yasset Perez-Riverol, Veit Schwämmle, Julian Uszkoreit, and Tim Van Den Bossche. "The European Bioinformatics Community for Mass Spectrometry (EuBIC-MS): An Open Community For Bioinformatics Training and Research." In: *Rapid Communications in Mass Spectrometry* (Apr. 16, 2021), e9087. DOI: 10.1002/rcm.9087.

[32] Samantha L Wilson, Gregory P Way, **Wout Bittremieux**, Jean-Paul Armache, Melissa A Haendel, and Michael M Hoffman. "Sharing Biological Data: Why, When, and How." In: *FEBS Letters* 595.7 (Apr. 2021), pp. 847–863. DOI: 10.1002/1873-3468.14067.

[31] **Wout Bittremieux**, Charlotte Adams, Kris Laukens, Pieter C Dorrestein, and Nuno Bandeira. "Open Science Resources for the Mass Spectrometry-Based Analysis of SARS-CoV-2." In: *Journal of Proteome Research* 20.3 (Mar. 5, 2021), pp. 1464–1475. DOI: 10.1021/acs.jproteome.0c00929.

[30] Pieter Moris, Joey De Pauw, Anna Postovskaya, Sofie Gielis, Nicolas De Neuter, **Wout Bittremieux**, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. "Current Challenges For Unseen-Epitope TCR Interaction Prediction and a New Perspective Derived From Image Classification." In: *Briefings in Bioinformatics* (Dec. 21, 2020), bbaa318. DOI: 10.1093/bib/bbaa318.

[29] Christopher Ashwood, **Wout Bittremieux**, Eric W Deutsch, Nadezhda T Doncheva, Viktoria Dorfer, Ralf Gabriels, Vladimir Gorshkov, Surya Gupta, Andrew R Jones, Lukas Käll, Dominik Kopczynski, Lydie Lane, Ludwig Lautenbacher, Marc Legeay, Marie Locard-Paulet, Bart Mesuere, Yasset Perez-Riverol, Eugen Netz, Julianus Pfeuffer, Timo Sachsenberg, Renee Salz, Patroklos Samaras, Henning Schiebenhoefer, Tobias Schmidt, Veit Schwämmle, Alessio Soggiu, Julian Uszkoreit, Tim Van Den Bossche, Bart Van Puyvelde, Joeri Van Strien, Pieter Verschaffelt, Henry Webel, and Sander Willems. "Proceedings of the EuBIC-MS 2020 Developers' Meeting." In: *EuPA Open Proteomics* 24 (Dec. 2020), pp. 1–6. DOI: 10.1016/j.euprot.2020.11.001.

[28] Alexander A Aksenov, Ivan Laponogov, Zheng Zhang, Sophie L F Doran, Ilaria Belluomo, Dennis Veselkov, **Wout Bittremieux**, Louis Felix Nothias, Mélissa Nothias-Esposito, Katherine N Maloney, Biswapriya B Misra, Alexey V Melnik, Aleksandr Smirnov, Xiuxia Du, Kenneth L Jones, Kathleen Dorrestein, Morgan Panitchpakdi, Madeleine Ernst, Justin J J van der Hooft, Mabel Gonzalez, Chiara Carazzone, Adolfo Amézquita, Chris Callewaert, James T Morton, Robert A Quinn, Amina Bouslimani, Andrea Albarracín Orio, Daniel Petras, Andrea M Smania, Sneha P Couvillion, Meagan C Burnet, Carrie D Nicora, Erika Zink, Thomas O Metz, Viatcheslav Artaev, Elizabeth Humston-Fulmer, Rachel Gregor, Michael M Meijler, Itzhak Mizrahi, Stav Eyal, Brooke Anderson, Rachel Dutton, Raphaël Lugan, Pauline Le Boulch, Yann Guitton, Stephanie Prevost, Audrey Poirier, Gaud Dervilly, Bruno Le Bizec, Aaron Fait, Noga Sikron Persi, Chao Song, Kelem Gashu, Roxana Coras, Monica Guma, Julia Manasson, Jose U Scher, Dinesh Kumar Barupal, Saleh Alseekh, Alisdair R Fernie, Reza Mirnezami, Vasilis Vasiliou, Robin Schmid, Roman S Borisov, Larisa N Kulikova, Rob Knight, Mingxun Wang, George B Hanna, Pieter C Dorrestein, and Kirill Veselkov. "Auto-Deconvolution and Molecular Networking of Gas Chromatography–Mass Spectrometry Data." In: *Nature Biotechnology* 39 (Nov. 9, 2020), pp. 169–173. DOI: 10.1038/s41587-020-0700-3.

[27] Sofie Gielis, Pieter Moris, **Wout Bittremieux**, Nicolas De Neuter, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. "Identification of Epitope-Specific T Cells in T-cell Receptor Repertoires." In: *Bioinformatics for Cancer Immunotherapy*. Ed. by Sebastian Boegel. Vol. 2120. New York, NY: Springer US, Mar. 3, 2020, pp. 183–195. DOI: 10.1007/978-1-0716-0327-7_13.

[26] Youzhong Liu, Aida Mrzic, Pieter Meysman, Thomas De Vijlder, Edwin P Romijn, Dirk Valkenborg, **Wout Bittremieux**, and Kris Laukens. "MESSAR: Automated Recommendation of Metabolite Substructures From Tandem Mass Spectra." In: *PLOS ONE* 15.1 (Jan. 16, 2020), e0226770. DOI: 10.1371/journal.pone.0226770.

[25] **Wout Bittremieux**. "spectrum_utils: A Python Package for Mass Spectrometry Data Processing and Visualization." In: *Analytical Chemistry* 92.1 (Jan. 7, 2020), pp. 659–661. DOI: 10.1021/acs.analchem.9b04884.

[24] Sofie Gielis, Pieter Moris, **Wout Bittremieux**, Nicolas De Neuter, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. "Detection of Enriched T Cell Epitope Specificity in Full T Cell Receptor Sequence Repertoires." In: *Frontiers in Immunology* 10 (Nov. 29, 2019), p. 2820. DOI: `10.3389/fimmu.2019.02820`.

[23] **Wout Bittremieux**, Kris Laukens, and William Stafford Noble. "Extremely Fast and Accurate Open Modification Spectral Library Searching of High-Resolution Mass Spectra Using Feature Hashing and Graphics Processing Units." In: *Journal of Proteome Research* 18.10 (Oct. 4, 2019), pp. 3792–3799. DOI: `10.1021/acs.jproteome.9b00291`.

[22] Lindsay Pino, Andy Lin, and **Wout Bittremieux**. "2018 YPIC Challenge: A Case Study in Characterizing an Unknown Protein Sample." In: *Journal of Proteome Research* 18.11 (Sept. 26, 2019), pp. 3936–3943. DOI: `10.1021/acs.jproteome.9b00384`.

[21] Pieter Meysman, Yvan Saeys, Ehsan Sabaghian, **Wout Bittremieux**, Yves van de Peer, Bart Goethals, and Kris Laukens. "Mining the Enriched Subgraphs for Specific Vertices in a Biological Graph." In: *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 16.5 (Sept. 2019), pp. 1496–1507. DOI: `10.1109/TCBB.2016.2576440`.

[20] Charlie Beirnaert, Laura Peeters, Pieter Meysman, **Wout Bittremieux**, Kenn Foubert, Deborah Custers, Anastasia Van der Auwera, Matthias Cuykx, Luc Pieters, Adrian Covaci, and Kris Laukens. "Using Expert Driven Machine Learning to Enhance Dynamic Metabolomics Data Analysis." In: *Metabolites* 9.3 (Mar. 20, 2019), p. 54. DOI: `10.3390/metabo9030054`.

[19] Dominik Kopczynski, **Wout Bittremieux**, David Bouyssié, Viktoria Dorfer, Marie Locard-Paulet, Bart Van Puyvelde, Veit Schwämmle, Alessio Soggiu, Sander Willems, and Julian Uszkoreit. "Proceedings of the EuBIC Winter School 2019." In: *EuPA Open Proteomics* 22–23 (Mar. 2019), pp. 4–7. DOI: `10.1016/j.euprot.2019.07.002`.

[18] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Journal of Proteome Research* 17.10 (Oct. 5, 2018), pp. 3463–3474. DOI: `10.1021/acs.jproteome.8b00359`.

[17] Sander Willems, David Bouyssié, Dieter Deforce, Viktoria Dorfer, Vladimir Gorshkov, Dominik Kopczynski, Kris Laukens, Marie Locard-Paulet, Veit Schwämmle, Julian Uszkoreit, Dirk Valkenborg, Marc Vaudel, and **Wout Bittremieux**. *Proceedings of the EuBIC Developer's Meeting 2018*. Sept. 15, 2018.

[16] Aida Mrzic, Pieter Meysman, **Wout Bittremieux**, Pieter Moris, Boris Cule, Bart Goethals, and Kris Laukens. "Grasping Frequent Subgraph Mining for Bioinformatics Applications." In: *BioData Mining* 11.20 (Sept. 3, 2018). DOI: `10.1186/s13040-018-0181-9`.

[15] **Wout Bittremieux**, David L Tabb, Francis Impens, An Staes, Evy Timmerman, Lennart Martens, and Kris Laukens. "Quality Control in Mass Spectrometry-Based Proteomics." In: *Mass Spectrometry Reviews* 37.5 (Sept. 2018), pp. 697–711. DOI: `10.1002/mas.21544`.

[14] Nicolas De Neuter, **Wout Bittremieux**, Charlie Beirnaert, Bart Cuypers, Aida Mrzic, Pieter Moris, Arvid Suls, Viggo Van Tendeloo, Benson Ogunjimi, Kris Laukens, and Pieter Meysman. "On the Feasibility of Mining CD8+ T-cell Receptor Patterns Underlying Immunogenic Peptide Recognition." In: *Immunogenetics* 70.3 (Mar. 2018), pp. 159–168. DOI: `10.1007/s00251-017-1023-5`.

[13] Eric W Deutsch, Sandra Orchard, Pierre-Alain Binz, **Wout Bittremieux**, Martin Eisenacher, Henning Hermjakob, Shin Kawano, Henry Lam, Gerhard Mayer, Gerben Menschaert, Yasset Perez-Riverol, Reza M Salek, David L Tabb, Stefan Tenzer, Juan Antonio Vizcaíno, Mathias Walzer, and Andrew R Jones. "Proteomics Standards Initiative: Fifteen Years of Progress and Future Work." In: *Journal of Proteome Research* 16.12 (Dec. 1, 2017), pp. 4288–4298. DOI: `10.1021/acs.jproteome.7b00370`.

[12] Juan Antonio Vizcaíno, Mathias Walzer, Rafael C Jiménez, **Wout Bittremieux**, David Bouyssié, Christine Carapito, Fernando Corrales, Myriam Ferro, Albert JR Heck, Peter Horvatovich, Martin Hubalek, Lydie Lane, Kris Laukens, Fredrik Levander, Frederique Lisacek, Petr Novak, Magnus Palmblad, Damiano Piovesan, Alfred Pühler, Veit Schwämmle, Dirk Valkenborg, Merlijn van Rijswijk, Jiri Vondrasek, Martin Eisenacher, Lennart Martens, and Oliver Kohlbacher. "A Community Proposal to Integrate Proteomics Activities in ELIXIR [Version 1; Referees: 2 Approved]." In: *F1000Research* 6 (June 13, 2017), p. 875. DOI: `10.12688/f1000research.11751.1`.

[11] **Wout Bittremieux**, Mathias Walzer, Stefan Tenzer, Weimin Zhu, Reza M Salek, Martin Eisenacher, and David L Tabb. "The Human Proteome Organization–Proteomics Standards Initiative Quality Control Working Group: Making Quality Control More Accessible for Biological Mass Spectrometry." In: *Analytical Chemistry* 89.8 (Apr. 18, 2017), pp. 4474–4479. DOI: `10.1021/acs.analchem.6b04310`.

[10] **Wout Bittremieux**, Dirk Valkenborg, Lennart Martens, and Kris Laukens. "Computational Quality Control Tools For Mass Spectrometry Proteomics." In: *PROTEOMICS* 17.3-4 (Feb. 2017), p. 1600159. DOI: `10.1002/pmic.201600159`.

[9] Evelyne Maes, Pieter Kelchtermans, **Wout Bittremieux**, Kurt De Grave, Sven Degroeve, Jef Hooyberghs, Inge Mertens, Geert Baggerman, Jan Ramon, Kris Laukens, Lennart Martens, and Dirk Valkenborg. "Designing Biomedical Proteomics Experiments: State-of-the-Art and Future Perspectives." In: *Expert Review of Proteomics* 13.5 (Apr. 25, 2016), pp. 495–511. DOI: `10.1586/14789450.2016.1172967`.

[8] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Dirk Valkenborg, and Kris Laukens. "Unsupervised Quality Assessment of Mass Spectrometry Proteomics Experiments by Multivariate Quality Control Metrics." In: *Journal of Proteome Research* 15.4 (Apr. 1, 2016), pp. 1300–1307. DOI: `10.1021/acs.jproteome.6b00028`.

[7] Pieter Meysman, Yvan Saeys, Ehsan Sabaghian, **Wout Bittremieux**, Yves Van de Peer, Bart Goethals, and Kris Laukens. "Discovery of Significantly Enriched Subgraphs Associated With Selected Vertices in a Single Graph." In: *Proceedings of the 14th International Workshop on Data Mining in Bioinformatics - BIOKDD '15*. Sydney, Australia, Aug. 10, 2015, p. 8.

[6] **Wout Bittremieux**, Hanny Willems, Pieter Kelchtermans, Lennart Martens, Kris Laukens, and Dirk Valkenborg. "iMonDB: Mass Spectrometry Quality Control through Instrument Monitoring." In: *Journal of Proteome Research* 14.5 (May 1, 2015), pp. 2360–2366. DOI: `10.1021/acs.jproteome.5b00127`.

[5] Stefan Naulaerts, Pieter Meysman, **Wout Bittremieux**, Trung Nghia Vu, Wim Vanden Berghe, Bart Goethals, and Kris Laukens. "A Primer to Frequent Itemset Mining For Bioinformatics." In: *Briefings in Bioinformatics* 16.2 (Mar. 2015), pp. 216–231. DOI: `10.1093/bib/bbt074`.

[4] Trung Nghia Vu, **Wout Bittremieux**, Dirk Valkenborg, Bart Goethals, Filip Lemière, and Kris Laukens. "Efficient Reduction of Candidate Matches in Peptide Spectrum Library Searching Using the Top k Most Intense Peaks." In: *Journal of Proteome Research* 13.9 (Sept. 5, 2014), pp. 4175–4183. DOI: `10.1021/pr401269z`.

[3] Mathias Walzer, Lucia Espona Pernas, Sara Nasso, **Wout Bittremieux**, Sven Nahnsen, Pieter Kelchtermans, Peter Pichler, Henk W P van den Toorn, An Staes, Jonathan Vandenbussche, Michael Mazanek, Thomas Taus, Richard A Scheltema, Christian D Kelstrup, Laurent Gatto, Bas van Breukelen, Stephan Aiche, Dirk Valkenborg, Kris Laukens, Kathryn S Lilley, Jesper Velgaard Olsen, Albert J R Heck, Karl Mechtler, Ruedi Aebersold, Kris Gevaert, Juan Antonio Vizcaino, Henning Hermjakob, Oliver Kohlbacher, and Lennart Martens. "qcML: An Exchange Format for Quality Control Metrics from Mass Spectrometry Experiments." In: *Molecular & Cellular Proteomics* 13.8 (Aug. 1, 2014), pp. 1905–1913. DOI: `10.1074/mcp.M113.035907`.

[2] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, and Kris Laukens. "jqcML: An Open-Source Java API for Mass Spectrometry Quality Control Data in the qcML Format." In: *Journal of Proteome Research* 13.7 (July 3, 2014), pp. 3484–3487. DOI: `10.1021/pr401274z`.

[1] Pieter Kelchtermans, **Wout Bittremieux**, Kurt De Grave, Sven Degroeve, Jan Ramon, Kris Laukens, Dirk Valkenborg, Harald Barsnes, and Lennart Martens. "Machine Learning Applications in Proteomics Research: How the Past Can Boost the Future." In: *PROTEOMICS* 14.4-5 (Mar. 2014), pp. 353–366. DOI: `10.1002/pmic.201300289`.

Other Manuscripts

[9] Issar Arab, Kris Laukens, and **Wout Bittremieux**. "Semi-Supervised Learning to Boost Cardiotoxicity Prediction by Mining a Large Unlabeled Small Molecule Dataset." In: *bioRxiv* (May 30, 2024). DOI: `10.1101/2024.05.25.595894`.

[8] **Wout Bittremieux**, Varun Ananth, William E. Fondrie, Carlo Melendez, Marina Pominova, Justin Sanders, Bo Wen, Melih Yilmaz, and William Stafford Noble. "Deep Learning Methods For De Novo Peptide Sequencing." In: *ChemRxiv* (May 27, 2024). DOI: `10.26434/chemrxiv-2024-l6wnt`.

[7] Carlo Melendez, Justin Sanders, Melih Yilmaz, **Wout Bittremieux**, Will Fondrie, Sewoong Oh, and William Stafford Noble. "Accounting for Digestion Enzyme Bias in Casanovo." In: *bioRxiv* (May 21, 2024). DOI: `10.1101/2024.05.16.594602`.

[6] Ceder Dens, Charlotte Adams, Kris Laukens, and **Wout Bittremieux**. "Machine Learning Strategies to Tackle Data Challenges in Mass Spectrometry-Based Proteomics." In: *bioRxiv* (May 5, 2024). DOI: `10.1101/2024.05.02.592141`.

[5] **Wout Bittremieux**. "From Data to Discovery: The Essential Role of Computational Tools in Proteomics." In: *PROTEOMICS* 24.8 (Apr. 2024), p. 2300081. DOI: `10.1002/pmic.202300081`.

[4] Janne Heirman and **Wout Bittremieux**. "Reusability Report: Annotating Metabolite Mass Spectra With Domain-Inspired Chemical Formula Transformers." In: *ChemRxiv* (Mar. 13, 2024). DOI: `10.26434/chemrxiv-2024-97r5j`.

[3] Ceder Dens, Kris Laukens, Pieter Meysman, and **Wout Bittremieux**. "A Cross-Attention Transformer Encoder For Paired Sequence Data." In: *bioRxiv* (Dec. 12, 2023). DOI: `10.1101/2023.12.11.571066`.

[2] Alan K. Jarmusch, Allegra T. Aron, Daniel Petras, Vanessa V. Phelan, **Wout Bittremieux**, Deepa D. Acharya, Mohammed M. A. Ahmed, Anelize Bauermeister, Matthew J. Bertin, Paul D. Boudreau, Ricardo M. Borges, Benjamin P. Bowen, Christopher J. Brown, Fernanda O. Chagas, Kenneth D. Clevenger, Mario S. P. Correia, William J. Crandall, Max Crüsemann, Tito Damiani, Oliver Fiehn, Neha Garg, William H Gerwick, Jeffrey R. Gilbert, Daniel Globisch, Paulo Wender P. Gomes, Steffen Heuckeroth, C. Andrew James, Scott A. Jarmusch, Sarvar A. Kakhkhorov, Kyo Bin Kang, Roland D Kersten, Hyunwoo Kim, Riley D. Kirk, Oliver Kohlbacher, Eftychia E. Kontou, Ken Liu, Itzel Lizama-Chamu, Gordon T. Luu, Tal Luzzatto Knaan, Michael T. Marty, Andrew C. McAvoy, Laura-Isobel McCall, Osama G. Mohamed, Omri Nahor, Timo H.J. Niedermeyer, Trent R. Northen, Kirsten E. Overdahl, Tomáš Pluskal, Johannes Rainer, Raphael Reher, Elys Rodriguez, Timo T. Sachsenberg, Laura M. Sanchez, Robin Schmid, Cole Stevens, Zhenyu Tian, Ashootosh Tripathi, Hiroshi Tsugawa, Kozo Nishida, Yuki Matsuzawa, Justin J.J. van der Hooft, Andrea Vicini, Axel Walter, Tilmann Weber, Quanbo Xiong, Tao Xu, Haoqi Nina Zhao, Pieter C. Dorrestein, and Mingxun Wang. "A Universal Language for Finding Mass Spectrometry Data Patterns." In: *bioRxiv* (Aug. 7, 2022). DOI: `10.1101/2022.08.06.503000`.

[1] **Wout Bittremieux**, Christopher Chen, Pieter C Dorrestein, Emma L Schymanski, Tobias Schulze, Steffen Neumann, Rene Meier, Simon Rogers, and Mingxun Wang. "Universal MS/MS Visualization and Retrieval with the Metabolomics Spectrum Resolver Web Service." In: *bioRxiv* (Sept. 26, 2020). DOI: `10.1101/2020.05.09.086066`.

Invited/Keynote Presentations

[6] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *HUPO Annual Conference* Cancun, Mexico (Dec. 7, 2022).

[5] **Wout Bittremieux**. "Introduction to Machine Learning." In: *Imaging Mass Spectrometry Workshop, ASMS Annual Conference* Minneapolis, MN, USA (June 7, 2022).

[4] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *Best of US HUPO 2022* (May 3, 2022). DOI: `10.5281/ZENODO.6515099`.

[3] **Wout Bittremieux**, Nicole Avalon, Sydney P. Thomas, Mingxun Wang, and Pieter C. Dorrestein. "Leveraging Public Untargeted Metabolomics Data to Propagate Structurally Related Molecule Annotations to Millions of MS/MS Spectra." In: *Applied Bioinformatics in Life Sciences* Leuven, Belgium (Mar. 11, 2022). DOI: `10.5281/ZENODO.6346949`.

[2] **Wout Bittremieux**. "Shedding Light on Complex Mass Spectrometry Proteomics Processes through Advanced Data Mining." In: *Faculty of Science Research Day* Antwerp, Belgium (Jan. 13, 2017). DOI: `10.5281/zenodo.242392`.

[1] **Wout Bittremieux** and Dirk Valkenborg. "iMonDB: Mass Spectrometry Instrument Monitoring for Quality Control." In: *Methods and Tools for Intra- and Inter-experiment LC MS Performance Tracking Workshop, ASMS Annual Conference* St. Louis, MO, USA (June 1, 2015).

Oral Presentations

[12] **Wout Bittremieux**, Damon H. May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *US HUPO 2022* Charleston, SC, USA (Mar. 1, 2022). DOI: `10.5281/ZENODO.6320843`.

[11] **Wout Bittremieux**, Julia Gauglitz, Alexander Aksenov, Alan K Jarmusch, Louis-Felix Nothias, Daniel Petras, Mingxun Wang, and Pieter C Dorrestein. "Repository-Scale Propagated Spectral Library of Suspects." In: *SoCal Science @Home Lollapalooza* (Dec. 1, 2020). DOI: `10.5281/zenodo.4300710`.

[10] **Wout Bittremieux**, Damon H May, Jeffrey Bilmes, and William Stafford Noble. "Deep Neural Network Embedding for Efficient Repository-Scale Analysis of Hundreds of Millions of Mass Spectra." In: *ASMS 2020 Reboot* (June 8, 2020). DOI: `10.5281/zenodo.3831052`.

[9] **Wout Bittremieux**, Kris Laukens, and William Stafford Noble. "Identifying Millions of Protein Modifications Using GPU-powered Approximate Nearest Neighbor Searching." In: *GPU Technology Conference* (Mar. 26, 2020). DOI: `10.5281/zenodo.3831055`.

[8] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Cascadia Proteomics Symposium* Seattle, WA, USA (July 23, 2018). DOI: `10.5281/zenodo.1319035`.

[7] **Wout Bittremieux**. "Git: How Version Control Can Power Your Research." In: *Biomina Lunch Talks* Antwerp, Belgium (June 24, 2016). DOI: `10.5281/zenodo.56352`.

[6] **Wout Bittremieux**, Dirk Valkenborg, and Kris Laukens. "Optimized Open Modification Spectral Library Searching Using Approximate Nearest Neighbor Techniques." In: *ASMS Annual Conference* San Antonio, TX, USA (June 9, 2016). DOI: `10.5281/zenodo.55999`.

[5] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Bart Goethals, Dirk Valkenborg, and Kris Laukens. "Approaches for Mass Spectrometry Quality Control." In: *Biomina Research Day* Antwerp, Belgium (Dec. 9, 2015). DOI: `10.5281/zenodo.56004`.

[4] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Bart Goethals, Dirk Valkenborg, and Kris Laukens. "Analysis of Mass Spectrometry Quality Control Metrics." In: *Benelux Bioinformatics Conference* Antwerp, Belgium (Dec. 7, 2015). DOI: `10.5281/zenodo.56001`.

[3] **Wout Bittremieux** and Kris Laukens. "Precursor-Free and Fast Spectral Library Search Using Approximate Nearest Neighbor Techniques." In: *Benelux Bioinformatics Conference Student Council Symposium* Antwerp, Belgium (Dec. 6, 2015). DOI: `10.5281/zenodo.56002`.

[2] **Wout Bittremieux**, Emmanuel Müller, Dirk Valkenborg, Lennart Martens, Bart Goethals, and Kris Laukens. "Pattern Mining of Mass Spectrometry Quality Control Data." In: *Benelux Bioinformatics Conference* Luxembourg, Luxembourg (Dec. 9, 2014). DOI: `10.5281/zenodo.56000`.

[1] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, and Kris Laukens. "Collecting and Mining Mass Spectrometry Quality Control Data." In: *Biomina Research Day* Antwerp, Belgium (Feb. 20, 2014). DOI: `10.5281/zenodo.56003`.

Poster Presentations

[15] Charlotte Adams, Issar Arab, William E. Fondrie, Kurt Boonen, Kris Laukens, and **Wout Bittremieux**. "Semi-Supervised Rescoring For Open Modification Searching Reveals Protein Modifications During SARS-CoV-2 Infection." In: *HUPO Annual Conference* Cancun. Mexico (Dec. 6, 2022).

[14] **Wout Bittremieux**, Robin Schmid, Florian Huber, Justin J.J. van der Hooft, Mingxun Wang, and Pieter C. Dorrestein. "Comparison of Spectrum Similarity Measures for Discovery of Structurally Related Molecules." In: *ASMS Annual Conference* Minneapolis, MN, USA (June 8, 2022). DOI: `10.5281/ZENODO.6609002`.

[13] **Wout Bittremieux**, Nicole Avalon, Sydney P. Thomas, Mingxun Wang, and Pieter C. Dorrestein. "Leveraging Public Untargeted Metabolomics Data to Propagate Annotations to Millions of MS/MS Spectra." In: *US HUPO 2022* Charleston, SC, USA (Mar. 1, 2022). DOI: `10.5281/ZENODO.6303580`.

[12] **Wout Bittremieux**, Sydney P Thomas, Mingxun Wang, and Pieter C Dorrestein. "Repository Scale Propagated Spectral Library of Suspects for Untargeted Metabolomics." In: *ASMS Annual Conference* Philadelphia, PA, USA (Nov. 2, 2021). DOI: `10.5281/ZENODO.5609253`.

[11] **Wout Bittremieux**, Damon H May, Jeffrey Bilmes, and William Stafford Noble. "A Learned Embedding for Efficient Joint Analysis of Millions of Mass Spectra." In: *Machine Learning in Computational Biology* Vancouver, BC, Canada (Dec. 14, 2019). DOI: `10.5281/zenodo.3576516`.

[10] **Wout Bittremieux**, Kris Laukens, and William Stafford Noble. "ANN-SoLo: Extremely Fast and Accurate Open Modification Spectral Library Searching." In: *ASMS Annual Conference* Atlanta, GA, USA (June 3, 2019). DOI: `10.5281/zenodo.3242687`.

[9] **Wout Bittremieux**, Pieter Meysman, William Stafford Noble, and Kris Laukens. "Fast Open Modification Spectral Library Searching through Approximate Nearest Neighbor Indexing." In: *Department of Genome Sciences Retreat* Leavenworth, WA, USA (Sept. 17, 2018). DOI: `10.5281/zenodo.1418397`.

[8] **Wout Bittremieux**, Dirk Valkenborg, and Kris Laukens. "Towards the Smart Lab: A Comprehensive Approach to Mass Spectrometry Quality Control." In: *ASMS Annual Conference* Indianapolis, IN, USA (June 8, 2017). DOI: `10.5281/zenodo.584052`.

[7] **Wout Bittremieux** and Kris Laukens. "Mass Spectrometry Proteomics: Ready for the Deep Learning (r)Evolution?" In: *ASMS Annual Conference* Indianapolis, IN, USA (June 8, 2017). DOI: `10.5281/zenodo.584067`.

[6] **Wout Bittremieux**, Pieter Meysman, Lennart Martens, Dirk Valkenborg, and Kris Laukens. "Automatic Quality Assessment of Mass Spectrometry Experiments by Multivariate Quality Control Metrics." In: *ASMS Annual Conference* San Antonio, TX, USA (June 9, 2016). DOI: `10.5281/zenodo.55998`.

[5] **Wout Bittremieux**, Hanny Willems, Lennart Martens, Dirk Valkenborg, and Kris Laukens. "Mass Spectrometry Quality Control: Instrument Monitoring and Pattern Mining Insights." In: *ASMS Annual Conference* St. Louis, MO, USA (June 2, 2015). DOI: `10.5281/zenodo.55992`.

[4] **Wout Bittremieux**, Hanny Willems, Lennart Martens, Bart Goethals, Dirk Valkenborg, and Kris Laukens. "A Comprehensive Approach to Mass Spectrometry Quality Control." In: *Two-day Symposium of the Belgian Proteomics Association* Brussels, Belgium (Dec. 18, 2014). DOI: `10.5281/zenodo.55990`.

[3] **Wout Bittremieux**, Dirk Valkenborg, Aida Mrzic, Hanny Willems, Bart Goethals, and Kris Laukens. "Pattern Mining of Mass Spectrometry Quality Control Data." In: *European Conference on Computational Biology* Strasbourg, France (Sept. 7, 2014). DOI: `10.5281/zenodo.55989`.

[2] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, Bart Goethals, and Kris Laukens. "Mining Mass Spectrometry Quality Control Data." In: *ASMS Annual Conference* Baltimore, MD, USA (June 16, 2014). DOI: `10.5281/zenodo.55988`.

[1] **Wout Bittremieux**, Pieter Kelchtermans, Dirk Valkenborg, Lennart Martens, and Kris Laukens. "jqcML: An Open-Source Java API for Mass Spectrometry Quality Control Data in the qcML Format." In: *Benelux Bioinformatics Conference* Brussels, Belgium (Dec. 9, 2013). DOI: `10.5281/zenodo.55986`.

Scientific Software Contributions

ANN-SoLo: A spectral library search engine for fast and accurate open modification searching.
    Homepage: `https://github.com/bittremieux/ANN-SoLo`
    Role: creator and maintainer
falcon: A tool for efficient clustering of millions of mass spectra.
    Homepage: `https://github.com/bittremieux/falcon`
    Role: creator and maintainer

GLEAMS: A deep neural network to convert mass spectrometry data to vector embeddings.
Homepage: https://github.com/bittremieux/GLEAMS
Role: creator and maintainer

iMonDB: A tool to automatically extract, store, manage, and visualize mass spectrometer instrument parameters from raw data files.
Homepage: https://github.com/bittremieux/iMonDB
Role: creator and maintainer

jqcML: A Java API for the qcML file format for mass spectrometry quality control data.
Homepage: https://github.com/bittremieux/jqcML
Role: creator and maintainer

Metabolomics USI: A web tool for FAIR mass spectrometry data.
Homepage: https://metabolomics-usi.gnps2.org/
Role: creator and maintainer

spectrum_utils: A Python package for efficient MS/MS spectrum processing and visualization.
Homepage: https://github.com/bittremieux/spectrum_utils
Role: creator and maintainer

Casanovo: *De novo* mass spectrometry peptide sequencing with a transformer deep neural network.
Homepage: https://github.com/Noble-Lab/casanovo
Role: contributor

DepthCharge: A deep learning toolkit for building state-of-the-art models in mass spectrometry.
Homepage: https://github.com/wfondrie/depthcharge
Role: contributor

GNPS: A web-based mass spectrometry ecosystem for untargeted metabolomics.
Homepage: https://gnps.ucsd.edu/
Role: contributor

ppx: A Python package for programmatic access to proteomics data repositories.
Homepage: https://github.com/wfondrie/ppx
Role: contributor

TCRex: A web tool for predicting TCR–epitope binding for human T cell receptors.
Homepage: https://tcrex.biodatamining.be/
Role: contributor

Student Supervision

2024–...   **Alejandro Mendoza Cantu**, PhD student
PhD thesis: *Reference Data-Driven Metabolomics to Study the Molecular Composition of South African foods*
Computer Science; University of Antwerp, Antwerp, Belgium

2024–...   **Marina Pominova**, PhD student
PhD thesis: *Computational Mass Spectrometry and Artificial Intelligence to Unravel the Immunopeptidome*
Computer Science; University of Antwerp, Antwerp, Belgium

2023–...   **Madina Bekbergenova**, PhD student
PhD thesis: *Deep Reinforcement Learning for Mass Spectrometry Data Acquisition in Metabolomics*
Computer Science; University of Antwerp, Antwerp, Belgium

2023–...   **Janne Heirman**, PhD student
PhD thesis: *Bioinformatics and Machine Learning For Large-Scale Metabolomics Data Analysis*
Computer Science; University of Antwerp, Antwerp, Belgium

2022–...   **Issar Arab**, PhD student
PhD thesis: *Open Modification Search Methods for Tandem Mass Spectrometry*
Computer Science; University of Antwerp, Antwerp, Belgium

2020–…	**Ceder Dens**, PhD student PhD thesis: *Artificial Intelligence to Decode the Peptide Sequences Driving the Immune Response* Computer Science; University of Antwerp, Antwerp, Belgium
2020–…	**Charlotte Adams**, PhD student PhD thesis: *Unraveling the Role of Protein Post-Translational Modifications During Viral Infection by Large-Scale Reprocessing of Open Mass Spectrometry-Based Interactome* Computer Science; University of Antwerp, Antwerp, Belgium
2024	**Michel Dierckx**, MSc student Internship: *Exploring the Evolutionary Presence of Post-Translational Modifications Through Public Mass Spectrometry-Based Proteomics Data Reanalysis* Computer Science; University of Antwerp, Antwerp, Belgium
2024	**Viktor Hura**, MSc student MSc thesis: *Machine Learning-Based Prediction of VCD Spectra For Molecular Mirror Images* Computer Science; University of Antwerp, Antwerp, Belgium
2024	**Cédric Leclercq**, MSc student MSc thesis: *Uncovering Maternal Drug Exposure Through Positive-Unlabeled Learning of Breast Milk Metabolomics* Computer Science; University of Antwerp, Antwerp, Belgium
2024	**Dzhem Myumyun**, MSc student MSc thesis: *AI-Driven ECG Pattern Recognition For Inherited Cardiac Arrhythmia and Cardiomyopathy* Computer Science; University of Antwerp, Antwerp, Belgium
2024	**Mathieu Maessen**, MSc student MSc thesis: *Exploring the Evolutionary Presence of Post-Translational Modifications Through Public Mass Spectrometry-Based Proteomics Data Reanalysis* Biomedical Sciences; University of Antwerp, Antwerp, Belgium
2021	**Lies Van Olmen**, MSc student MSc thesis: *Identification of Post-Translational Modifications in Epitopes* Biotechnology; University of Antwerp, Antwerp, Belgium
2020	**Jens Settelmeier**, MSc student MSc thesis: *Deep Neural Embedding of Chimeric Tandem Mass Spectra* Machine Learning; Royal Institute of Technology, Stockholm, Sweden
2019	**Charlotte Adams**, MSc student MSc thesis: *Deep Reprocessing of Mass Spectrometry-Based Human and Virus-Host Protein Interaction Data Using Open Modification Searching* Biotechnology; University of Antwerp, Antwerp, Belgium
2019	**Charlotte Adams**, MSc student Internship: *Investigating the Advantages of Open Modification Searching to Identify Modified Proteins* Biotechnology; University of Antwerp, Antwerp, Belgium
2019	**Stephen Blaskowski**, PhD student Internship: *Using Machine Learning to Speed Up Calibration of Tandem Mass Spectrometry Database Search* Molecular Engineering; University of Washington, Seattle, WA, USA
2017	**Joeri Reyns**, MSc student MSc thesis: *Protein Identification Using Deep Neural Networks* Computer Science; University of Antwerp, Antwerp, Belgium
2017	**Keerthana Sanala Prakash**, MSc student Internship: *Temporal Mining of Mass Spectrometry Quality Control Data* Computer Science; University of Antwerp, Antwerp, Belgium
2016	**Phui San Cheong**, MSc student Internship: *Implement Frequent Itemset-based Clustering in pyGCluster* Computer Science; University of Antwerp, Antwerp, Belgium

2016	**Robin Verachtert**, BSc student
	Internship: *Automatic Discovery of Artefacts in Mass Spectrometry Data*
	Computer Science; University of Antwerp, Antwerp, Belgium

Teaching

Training

2022	The Carpentries Instructor Training

Experience

2024–…	Biomedical Artificial Intelligence: Instructor, University of Antwerp – Master of Computer Science
2024–…	Machine Learning: Instructor, University of Antwerp – Master Biochemistry and Biotechnology
2024–…	Introduction to Computational Biology: Instructor, University of Antwerp – Bachelor of Computer Science
2022–…	Fundamentals of Machine Learning for Mass Spectrometry Data Analysis: Instructor, American Society for Mass Spectrometry – Annual Conference Short Course
2021	System-Wide Mass Spectrometry: Guest Lecturer, University of California San Diego – Cellular & Molecular Medicine
2017	Introduction to Computational Biology: Teaching Assistant, University of Antwerp – Bachelor of Computer Science
2016	Project Work: Teaching Assistant, University of Antwerp – Bachelor of Mathematics
2014–15	Data Mining: Teaching Assistant, University of Antwerp – Master of Biochemistry and Biotechnology
2015	Data Mining: Guest Lecturer, University of Antwerp – Master of Computer Science

Funding Acquired

Current Support

BOF 23-AWP-COE-11 (Covaci)	2026/01/01 – 2031/12/31
University of Antwerp – University Research Fund	€720,000

Exposomics: A Holistic Approach to Assess Environmental Exposures and Their Impact on Endocrine and Metabolic Disorders
Role: Co-PI

FWO 12A4025N (Bittremieux)	2024/10/01 – 2027/09/30
Research Foundation – Flanders	€332,940

Deep Learning For Comprehensive Small Molecule Discovery From Untargeted Mass Spectrometry Data
Role: PI

IOF POC CREATE 51155 (Bittremieux)	2024/05/01 – 2025/05/30
University of Antwerp – Industrial Research Fund	€125,000

De Novo Mass Spectrometry Peptide Sequencing With a Transformer Large Language Model
Role: PI

FWO G0AGQ24N (Bittremieux)   2024/01/01 – 2026/12/31
Research Foundation – Flanders   €314,450
Reference Data-Driven Metabolomics to Study the Molecular Composition of South African Foods
Role: PI

FWO W000924N (Bittremieux)   2024/01/01 – 2028/12/31
Research Foundation – Flanders   €60,000
Bioinformatics Network For Proteomics and Mass Spectrometry
Role: PI

SPECTRUM (Nothias)   2023/12/01 – 2026/11/30
University of the Côte d'Azur
Deep Reinforcement Learning for Mass Spectrometry Data Acquisition in Metabolomics
Role: Co-PI

BOF 49083-DOCPRO2023 (Bittremieux)   2023/10/01 – 2027/09/30
University of Antwerp – University Research Fund   €245,000
Computational Mass Spectrometry and Artificial Intelligence to Unravel the Immunopeptidome
Role: PI

POC-PP 49336 (Laukens)   2023/05/01 – 2024/12/31
Plan Flemish Resilience – Infectious Diseases & Environmental Health   €161,423
Enabling Mobile and Data-Driven Pathogen Monitoring Through a Paired Nanopore Squiggle–Genome Sequence Database
Role: Co-PI

BOF 49298-DOCPRO2022 (Bittremieux)   2022/12/01 – 2026/11/30
University of Antwerp – University Research Fund   €225,000
Bioinformatics and Machine Learning For Large-Scale Metabolomics Data Analysis
Role: PI

Previous Support

NIH 1R03OD034493-01 (Dorrestein)   2022/09/01 – 2023/08/31
National Institutes of Health $302,764
Cross Repository Metabolomics Data and Workflow Integration
Role: Co-Investigator

BOF 40004-DOCPRO2019 (Laukens)   2019/10/01 – 2023/09/30
University of Antwerp – University Research Fund   €205,000
Transferable Deep Learning for Sequence Based Prediction of Molecular Interactions
Role: Co-PI

BAEF 2017-FELLOW-E060 (Bittremieux)   2018/07/01 – 2019/06/30
Belgian American Educational Foundation $45,000
Prediction of Mass Spectrometry Spectral Libraries
Role: Postdoctoral Fellow

FWO 12W0418N (Bittremieux)   2017/10/01 – 2020/07/31
Research Foundation – Flanders   €265,300
Intelligent Quality Control for Mass Spectrometry-based Proteomics
Role: Postdoctoral Fellow

Professional Activities

Referee

Journals   Analytical Chemistry, Artificial Intelligence in Medicine, Bioinformatics, BMC Bioinformatics, Communications Biology, Genome Biology, IEEE/ACM Transactions on Computational Biology and Bioin-

formatics, Journal of the American Society for Mass Spectrometry, Journal of Computational Biology, Journal of Open Source Software, Journal of Proteome Research, Mass Spectrometry Reviews, Metabolites, Nature Biotechnology, Nature Communications, Nature Machine Intelligence, PLOS Computational Biology, PLOS ONE, PROTEOMICS, Scientific Reports

Conferences   European Conference on Computational Biology (ECCB), Intelligent Systems for Molecular Biology (ISMB), Machine Learning in Computational Biology (MLCB), NIPS Workshop on Machine Learning in Computational Biology, Research in Computational Molecular Biology (RECOMB), Workshop on Data Mining in Bioinformatics (BIOKDD)

Editor

Guest editor for PLOS Computational Biology and PROTEOMICS.

Scientific Meetings Organized

2025	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Neustift, Italy): Organizing Committee Member
2024	National Synthesis Center for Emergence in the Molecular and Cellular Sciences Summit Meeting (Chicago, IL, USA): Thematic Chair
2024	European Bioinformatics Community for Mass Spectrometry – ProteoBench Workshop (Ghent, Belgium): Main Organizer
2024	Intelligent Systems for Molecular Biology (Montreal, QC, Canada) – Computational Mass Spectrometry Track: Chair
2023	Intelligent Systems for Molecular Biology / European Conference on Computational Biology (Lyon, France) – Computational Mass Spectrometry Track: Chair
2022	Intelligent Systems for Molecular Biology (Madison, WI, USA) – Computational Mass Spectrometry Track: Chair
2022	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Oeiras, Portugal): Organizing Committee Member
2022	US HUPO Annual Conference (Charleston, SC, USA) – Computational Proteomics: From Machine Learning to Human Insight Track: Chair
2021	American Society for Mass Spectrometry Annual Conference (Philadelphia, PA, USA) – Quality Control Workshop: Chair
2021	Intelligent Systems for Molecular Biology / European Conference on Computational Biology (online) – Computational Mass Spectrometry Track: Chair
2020	Intelligent Systems for Molecular Biology Conference (online) – Computational Mass Spectrometry Track: Co-chair
2020	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Nyborg, Denmark): Organizing Committee Member
2019	Machine Learning in Computational Biology (Vancouver, BC, Canada): Program Committee Member
2019	European Bioinformatics Community for Mass Spectrometry Winter School (Zakopane, Poland): Organizing Committee Member
2018	European Bioinformatics Community for Mass Spectrometry Developers' Meeting (Ghent, Belgium): Main Organizer
2015	Benelux Bioinformatics Community (Antwerp, Belgium): Organizing Committee Member
2014	Belgian Proteomics Association Symposium (Brussels, Belgium): Local Organizing Committee Member

Professional Affiliations

2022–…   Human Proteome Organization – Proteomics Standards Initiative: Chair of the Quality Control Working Group
2021–…   Human Proteome Organization: Member
2017–…   European Bioinformatics Community for Mass Spectrometry: Member
2016–2022   Human Proteome Organization – Proteomics Standards Initiative: Secretary of the Quality Control Working Group
2014–…   International Society for Computational Biology: Member
2013–…   Belgian Proteomics Association: Member
2013–…   American Society for Mass Spectrometry: Member